Asymptotics for the Eigenvalues of the Harmonic Oscillator with a Quasi-Periodic Perturbation

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Abstract

We consider operators of the form $H+V$ where H is the one-dimensional harmonic oscillator and V is a zero-order pseudo-differential operator which is quasi-periodic in an appropriate sense (one can take V to be multiplication by a periodic function for example). It is shown that the eigenvalues of $H+V$ have asymptotics of the form $\lambda_n(H+V) = \lambda_n(H) + W(\sqrt{n})n^{-1/4} + O(n^{-1/2}\ln(n))$ as $n \to +\infty$, where W is a quasi-periodic function which can be defined explicitly in terms of V.

1 Introduction

The one-dimensional harmonic oscillator is the operator

$$H \;=\; -\frac{d^2}{dx^2} + (\alpha x)^2,$$

where α is a positive parameter. We can consider H as an unbounded self-adjoint operator acting on $L^2(\mathbb{R})$. The determination of the spectrum of H is a classical problem — virtually any introductory book on quantum mechanics has a section devoted to this topic. In particular H has a compact resolvent and hence a discrete spectrum. Furthermore, the eigenvalues of H are simple and can be enumerated as

$$\lambda_n(H) = \alpha(2n+1), \qquad n \in \mathbb{N}_0.$$

A normalised eigenfunction corresponding to $\lambda_n(H)$ can be chosen as

$$\phi_n(x) \;=\; \frac{\alpha^{1/4}}{\sqrt{n!\,2^n\sqrt{\pi}}}\, e^{-\alpha x^2/2}\, \mathcal{H}_n(\sqrt{\alpha}x), \tag{1}$$

where $\mathcal{H}_n$ is the n–th Hermite polynomial.

The purpose of this paper is to study the large n asymptotics of the eigenvalues of the perturbed operator $H+V$ when V is a self-adjoint quasi-periodic pseudo-differential operator of order 0. More precisely, we assume V can be written in the form

$$V \;=\; \sum_{\mathbf{a}\in\Lambda} V_{\mathbf{a}} U_{\mathbf{a}} \tag{2}$$

where $\Lambda \subset T^*\mathbb{R} \cong \mathbb{R}^2$ is a countable discrete index set and, for each $\mathbf{a} = (a_x, a_\xi) \in T^*\mathbb{R}$, we define $U_{\mathbf{a}}$ to be the unitary operator on $L^2(\mathbb{R})$ given by

$$U_{\mathbf{a}}\phi(x) \;=\; e^{ia_x a_\xi/2} e^{ia_x x}\phi(x+a_\xi). \tag{3}$$

The $V_{\mathbf{a}}$'s are just complex coefficients.

Since $U_{\mathbf{a}}^* = U_{-\mathbf{a}}$ for any $\mathbf{a} \in T^*\mathbb{R}$, the condition that V is self-adjoint can be rewritten as the requirement

$$\mathbf{a}\in\Lambda \implies -\mathbf{a}\in\Lambda \quad \text{and} \quad V_{-\mathbf{a}} = \overline{V_{\mathbf{a}}}, \quad \mathbf{a}\in\Lambda.$$

We will also assume the $V_{\mathbf{a}}$'s satisfy the following condition (essentially a regularity assumption);

$$\sum_{\mathbf{a}\in\Lambda} |\mathbf{a}|^3 |V_{\mathbf{a}}| \;<\; +\infty. \tag{4}$$

In particular, this condition ensures that the right hand side of (2) is absolutely convergent in operator norm, making V a well defined bounded operator. Since H has a compact resolvent the same must then be true for $H+V$; it follows that the spectrum of $H+V$ also consists of discrete eigenvalues.

Remark. If we take $\Lambda = \{(\omega m, 0)\,|\, m\in\mathbb{Z}\}$ then V is the operator of multiplication by a function with period ω whose m-th Fourier coefficient is simply $\omega^{1/2}V_{(\omega m,0)}$. Condition (4) becomes a standard regularity requirement (that the function V should be a "bit more" than C^3).

In general we may consider V to be a zero-order pseudo-differential operator with Weyl-symbol $\sum_{\mathbf{a}\in\Lambda} V_{\mathbf{a}} e^{i(a_x x + a_\xi \xi)}$ (n.b., $U_{\mathbf{a}}$ is the operator with Weyl-symbol $e^{i(a_x x+a_\xi\xi)}$). If Λ is a rational periodic lattice then V will be a periodic operator (in the sense that it commutes with a specific translation operator). Taking Λ to be an irrational periodic lattice, or an irregular discrete set, leads to a generalisation of such periodic operators; when we apply "quasi-periodic" to V we mean this particular type of generalisation.

If $\mathbf{0}\in\Lambda$ then the corresponding term in V is $V_{\mathbf{0}}$ times the identity operator and will thus cause a simple shift in the spectrum of H by $V_{\mathbf{0}}$. This term is included in the statement of the main result (Theorem 1.1 below) but thereafter we shall assume $V_{\mathbf{0}} = 0$. We also set $\Lambda' = \Lambda\backslash\{\mathbf{0}\}$; since Λ is discrete, $T^*\mathbb{R}\backslash\Lambda'$ contains a neighbourhood of $\mathbf{0}$.

Define a metric $|\cdot|_\alpha$ on $T^*\mathbb{R}$ by $|\mathbf{a}|_\alpha = (\alpha^{-1}a_x^2 + \alpha\, a_\xi^2)^{1/2}$. This metric is equivalent to the usual metric $|\cdot|$ so condition (4) can be rewritten as

$$\sum_{\mathbf{a}\in\Lambda'} |\mathbf{a}|_\alpha^p |V_\mathbf{a}| \;<\; +\infty \quad \text{for all } p \leq 3. \tag{5}$$

The main result of the paper is the following.

Theorem 1.1. *Suppose V given by* (2) *satisfies* (4) *(or equivalently* (5)*). Then the eigenvalues of the operator $H+V$ satisfy*

$$\lambda_n(H+V) \;=\; \alpha(2n{+}1) \;+\; V_\mathbf{0} \;+\; W(\sqrt{n})\,n^{-1/4} \;+\; O(n^{-1/2}\ln(n))$$

as $n \to \infty$, where $W : \mathbb{R} \to \mathbb{R}$ is the quasi-periodic function defined by

$$W(\lambda) \;=\; \frac{2^{1/4}}{\sqrt{\pi}} \sum_{\mathbf{a}\in\Lambda'} V_\mathbf{a} |\mathbf{a}|_\alpha^{-1/2} \cos\Bigl(\sqrt{2}\,|\mathbf{a}|_\alpha \lambda - \frac{\pi}{4}\Bigr). \tag{6}$$

The presence of the quasi-periodic function W means the first order asymptotics given by Theorem 1.1 contain considerably more information about the operator V than one might expect (c.f. the simple power type asymptotics for the case when V is given as multiplication by an element of C_0^∞ ([PS]) or for the operator $-d^2/d\theta^2{+}V(\theta)$ on S^1 (see Theorem 4.2 in [MO])). In particular we note that if V is given as multiplication by a periodic function, knowledge of the first order asymptotics of $\lambda_n(H+V)$ allows the Fourier coefficients of V to be "half" determined (the values of $V_{(-m\omega,0)} + V_{(m\omega,0)}$, $m \in \mathbb{N}$, can be determined from W).

It is likely that there exists a full asymptotic expansion for $\lambda_n(H+V)$, involving further terms with quasi-periodic functions multiplying increasingly negative powers of n. Judging by numerical evidence (for example with the potential $V(x) = \cos(x)$) the second term in the asymptotics is $O(n^{-3/4})$. This order (even as an improvement of the remainder estimate in Theorem 1.1) appears to involve reasonable subtle cancellation effects within the series giving the second term of the asymptotics; no attempt to deal with this analysis is made here.

Remark. With an obvious modification to the definition of W and a remainder estimate of $O(n^{-1/3}\ln(n))$, Theorem 1.1 also holds for operators V of the form

$$V \;=\; \int_{T^*\mathbb{R}} V_\mathbf{a} U_\mathbf{a}\, d^2\mathbf{a} \quad \text{where } V_\mathbf{a} \text{ satisfies} \quad \int_{T^*\mathbb{R}} (|\mathbf{a}|_\alpha^{-3/2} + |\mathbf{a}|_\alpha^3)|V_\mathbf{a}|\, d^2\mathbf{a} \;<\; +\infty.$$

In this case V is a pseudo-differential operator of order zero whose Weyl-symbol has Fourier transform $2\pi V_\mathbf{a}$. The $|\mathbf{a}|_\alpha^3$ term in the condition on $V_\mathbf{a}$ is then a regularity condition, while the $|\mathbf{a}|_\alpha^{-3/2}$ term is a generalisation of quasi-periodicity.

The proof of Theorem 1.1 is given in Section 4 using standard ideas to express the eigenvalues of $H+V$ in terms of a series involving the resolvent of H and the operator V. The non-triviality of Theorem 1.1 is contained in technical results used to establish the convergence of these series. These results are obtained in Sections 2 and 3; estimates for the elements $\langle V\phi_k, \phi_{k'}\rangle$ of the matrix of V with respect to the eigenbasis $\{\phi_k \,|\, k \in \mathbb{N}_0\}$ are obtained in the former and are then combined to give resolvent estimates in the latter.

Notation. We use C to denote any positive real constant whose exact value is not important but which may depend only on the things it is allowed to in a given problem. Appropriate function type notation is used in places to make this clearer whilst subscripts are added if we need to keep track of the value of a particular constant (e.g. $C_1(V)$ etc.).

We use $\|T\|$, $\|T\|_1$ and $\|T\|_2$ to denote the operator, trace class and Hilbert-Schmidt norms of the operator T respectively.

2 Estimates for Matrix Elements

The aim of this section is to obtain the necessary estimates for the matrix elements $\langle V\phi_k, \phi_{k'}\rangle$ for all $k, k' \in \mathbb{N}_0$. In turn these will be estimated via

$$U_{\mathbf{a}}^{k,k'} := \langle U_{\mathbf{a}}\phi_k, \phi_{k'}\rangle \tag{7}$$

defined for all $\mathbf{a} \in T^*\mathbb{R}$ and $k, k' \in \mathbb{N}_0$. Since the operator $U_{\mathbf{a}}$ is unitary we immediately get

$$|U_{\mathbf{a}}^{k,k'}| \leq 1. \tag{8}$$

To obtain more precise estimates we can use the following special function identity (see 7.377 on page 844 of [GRJ]) to find an explicit formula for $U_{\mathbf{a}}^{k,k'}$; for any $0 \leq k \leq k'$ and $y, z \in \mathbb{C}$ we have

$$\int_{\mathbb{R}} e^{-x^2}\mathcal{H}_k(x+y)\mathcal{H}_{k'}(x+z)\,dx = 2^{k'}\sqrt{\pi}\,k!\,z^{k'-k}L_k^{(k'-k)}(-2yz), \tag{9}$$

where $L_k^{(k'-k)}$ is the generalised Laguerre polynomial.

Lemma 2.1. *For any $0 \leq k \leq k'$ and $\mathbf{a} \in T^*\mathbb{R}\backslash\{\mathbf{0}\}$ we have*

$$U_{\mathbf{a}}^{k,k'} = \sqrt{\frac{k!}{k'!}}(\sqrt{2}\rho e^{i\theta})^{k'-k}\,e^{-\rho^2}\,L_k^{(k'-k)}(2\rho^2)$$

for some $\theta \in \mathbb{R}$, where

$$\rho = \frac{1}{2}\Big(\frac{a_x^2}{\alpha} + \alpha a_\xi^2\Big)^{1/2} = \frac{1}{2}|\mathbf{a}|_\alpha. \tag{10}$$

Proof. Introduce the complex number

$$\omega \;=\; \frac{\sqrt{\alpha}\, a_\xi}{2} - i\,\frac{a_x}{2\sqrt{\alpha}}.$$

From (7), (3) and (1) we get

$$\begin{aligned}
U_{\mathbf{a}}^{k,k'} &= \langle U_{\mathbf{a}}\phi_k, \phi_{k'}\rangle \\
&= \frac{\sqrt{\alpha}\,2^{-(k+k')/2}}{\sqrt{k!k'!\pi}} e^{ia_x a_\xi/2} \int_{\mathbb{R}} e^{ia_x x}\, e^{-\alpha(x+a_\xi)^2/2}\, e^{-\alpha x^2/2} \\
&\qquad\qquad \mathcal{H}_k(\sqrt{\alpha}(x+a_\xi))\, \mathcal{H}_{k'}(\sqrt{\alpha}\,x)\, dx \\
&= \frac{2^{-(k+k')/2}}{\sqrt{k!k'!\pi}}\, e^{\omega^2 - \alpha a_\xi^2/2 + ia_x a_\xi/2} \int_{\mathbb{R}} e^{-x^2}\, \mathcal{H}_k(x-\omega+\sqrt{\alpha}a_\xi)\, \mathcal{H}_{k'}(x-\omega)\, dx \\
&= \sqrt{\frac{k!}{k'!}}\, 2^{(k'-k)/2} (-\omega)^{k'-k} e^{\omega^2 - \alpha a_\xi^2/2 + ia_x a_\xi/2} L_k^{(k'-k)}\big(-2\omega(\omega - \sqrt{\alpha}\, a_\xi)\big)
\end{aligned}$$

where the last line follows from (9). Now $|\omega| = \rho$ while

$$\omega^2 - \frac{\alpha a_\xi^2}{2} + \frac{ia_x a_\xi}{2} \;=\; \frac{\alpha a_\xi^2}{4} - \frac{a_x^2}{4\alpha} - \frac{\alpha a_\xi^2}{2} - \frac{ia_x a_\xi}{2} + \frac{ia_x a_\xi}{2} \;=\; -|\omega|^2$$

and

$$-2\omega(\omega - \sqrt{\alpha}\, a_\xi) \;=\; -2\omega(-\overline{\omega}) \;=\; 2|\omega|^2.$$

The result follows. ∎

Throughout the remainder of this section we will assume $\mathbf{a} \in T^*\mathbb{R}\setminus\{\mathbf{0}\}$ is fixed and $\rho > 0$ is given by (10).

Laguerre polynomials can be expressed in terms of the confluent hypergeometric function; using 22.5.54 in [AS] we get

$$L_k^{(k'-k)}(2\rho^2) \;=\; \binom{k'}{k} M(-k, k'-k+1, 2\rho^2).$$

The confluent hypergeometric function can, in turn, be written as a pointwise absolutely convergent series of Bessel functions; from 13.3.7 in [AS] we get

$$\begin{aligned}
M(-k, k'-k+1, 2\rho^2) &= (k'-k)!\, e^{\rho^2} \big(\rho^2(k'+k+1)\big)^{-(k'-k)/2} \\
&\qquad \sum_{j=0}^{\infty} A_j \left(\frac{\rho}{(k'+k+1)^{1/2}}\right)^j J_{k'-k+j}\big(2\rho\sqrt{k'+k+1}\big),
\end{aligned}$$

where

$$A_0 = 1, \quad A_1 = 0, \quad A_2 = \frac{1}{2}(k'-k+1) \tag{11}$$

and, for $j \geq 2$,

$$(j+1)A_{j+1} \;=\; (j+k'-k)A_{j-1} - (k'+k+1)A_{j-2}. \tag{12}$$

It follows from Lemma 2.1 that

$$U_{\mathbf{a}}^{k,k'} \;=\; e^{i(k'-k)\theta}\sqrt{F_{k',k}}\,\sum_{j=0}^{\infty} A_j\left(\frac{\rho}{(k'+k+1)^{1/2}}\right)^j J_{k'-k+j}\big(2\rho\sqrt{k'+k+1}\big), \tag{13}$$

where

$$F_{k',k} \;:=\; \frac{k'!}{k!}\Big(\frac{2}{k'+k+1}\Big)^{k'-k}.$$

The next two results give estimates for the constants appearing in (13).

Lemma 2.2. *Suppose $k' \geq 2$ and $0 \leq k'-k \leq {k'}^{2/3}$. Then*

$$|A_j| \;\leq\; (k'+k+1)^{j/3}.$$

Proof. Set $m = k'-k$ and $n = k'+k+1$ so

$$0 \;\leq\; m \;\leq\; {k'}^{2/3} \;\leq\; (k'+k+1)^{2/3} \;=\; n^{2/3}$$

while $k' \geq 2$ and $k \geq 0$ so $n \geq 3$.

We have $A_0 = 1 = n^0$, $A_1 = 0 \leq n^{1/3}$ and $m, 1 \leq n^{2/3}$ so $A_2 = \frac{1}{2}(m+1) \leq n^{2/3}$. Now let $J \geq 2$ and suppose the result hold for $j \leq J$. Since

$$A_{J+1} \;=\; \frac{J+m}{J+1}A_{J-1} - \frac{n}{J+1}A_{J-2}$$

we then get

$$|A_{J+1}| \;\leq\; \frac{J+m}{J+1}n^{(J-1)/3} + \frac{n}{J+1}n^{(J-2)/3} \;=\; n^{(J+1)/3}\,\frac{(J+m)n^{-2/3}+1}{J+1}.$$

Now $mn^{-2/3} \leq 1$ while

$$\begin{aligned} n \geq 3 \;&\Longrightarrow\; n^{-2/3} \leq 3^{-2/3} \leq \tfrac{1}{2} \\ &\Longrightarrow\; J(1-n^{-2/3}) \geq 1 \qquad \text{(as } J \geq 2\text{)} \\ &\Longrightarrow\; 1 + Jn^{-2/3} \leq J. \end{aligned}$$

Thus $(J+m)n^{-2/3}+1 \leq J+1$. Therefore $|A_{J+1}| \leq n^{(J+1)/3}$ and the result follows by induction. ∎

Lemma 2.3. *If $0 \leq k \leq k'$ then $F_{k',k} \leq 1$.*

Proof. We have

$$F_{k',k} = \frac{k'(k'-1)\dots(k+1)}{\frac{1}{2}(k'+k+1)\dots\frac{1}{2}(k'+k+1)},$$

where the numerator and denominator both contain $k'-k$ terms. Now set $m = \frac{1}{2}(k'-k-1)$ and $n = \frac{1}{2}(k'+k+1)$ so $m \le n$ while

$$F_{k',k} = \frac{(n+m)}{n}\frac{(n+m-1)}{n}\dots\frac{(n-m-1)}{n}\frac{(n-m)}{n}.$$

If $k'-k$ is odd this can be rearranged as

$$F_{k',k} = \frac{(n+m)(n-m)}{n^2}\frac{(n+m-1)(n-m-1)}{n^2}\dots\frac{n}{n},$$

while if $k'-k$ is even we get

$$F_{k',k} = \frac{(n+m)(n-m)}{n^2}\frac{(n+m-1)(n-m-1)}{n^2}\dots\frac{(n+\frac{1}{2})(n-\frac{1}{2})}{n^2}.$$

The result now follows from the fact that

$$\frac{(n+m')(n-m')}{n^2} = \frac{n^2-m'^2}{n^2} \le 1$$

for any $0 \le m' \le n$. ■

Next we obtain some estimates for the Bessel functions appearing in (13).

Lemma 2.4. *For any $x, \varepsilon > 0$ and $n \in [0, x/2]$*

$$\left|\left\{\theta \in [0,\pi] \,\big|\, |x\cos(\theta) - n| < \varepsilon\right\}\right| \le \frac{4\pi}{3}\frac{\varepsilon}{x}.$$

Proof. Set $\delta = \varepsilon/x$, $y = n/x$ and $\Omega_{y,\delta} = \mathrm{Cos}^{-1}([y-\delta, y+\delta])$; we need to show that $|\Omega_{y,\delta}| \le 4\pi\delta/3$.

Now set $\theta_0 = \mathrm{Cos}^{-1}(y)$ and let $\ell(\theta)$ denote the affine function with $\ell(0) = 1$ and $\ell(\theta_0) = y$. It is easy to see that $|\cos(\theta) - y| \ge |\ell(\theta) - y|$ which implies $|\Omega_{y,\delta}| \le 2\delta/|L|$ where L is the gradient of $\ell(\theta)$. On the other hand, $y \in [0, \frac{1}{2}]$ so the minimum value for $|L|$ occurs when $y = 1/2$; hence $1/|L| \le 2\,\mathrm{Cos}^{-1}(1/2) = 2\pi/3$ and the result follows. ■

Lemma 2.5. *For any $n \in \mathbb{N}_0$ and $x \ge 2n$ we have $|J_n(x)| \le 4x^{-1/2}$.*

Surely this estimate (or an improvement) lies in a book somewhere!

Proof. Define a function by $f(\theta) = x\sin(\theta) - n\theta$ so we have the following integral representation for the Bessel function J_n (see 9.1.21 in [AS]);

$$J_n(x) \;=\; \frac{1}{\pi}\int_0^\pi \cos(f(\theta))\,d\theta. \tag{14}$$

Now set

$$\Omega_0 = \big\{\theta \in [0,\pi]\,\big|\,|f'(\theta)| < x^{1/2}\big\} \quad \text{and} \quad \Omega_1 = [0,\pi]\backslash\Omega_0$$

so $J_n(x) = (I_0 + I_1)/\pi$ where $I_k = \int_{\Omega_k}\cos(f(\theta))\,d\theta$ for $k = 0, 1$. Lemma 2.4 gives

$$|I_0| \;\le\; |\Omega_0| \;\le\; \frac{4\pi}{3}x^{-1/2}. \tag{15}$$

On the other hand

$$I_1 \;=\; \left[\frac{\sin(f(\theta))}{f'(\theta)}\right]_{\partial\Omega_1} + \int_{\Omega_1}\frac{f''(\theta)}{(f'(\theta))^2}\sin(f(\theta))\,d\theta.$$

Now $f''(\theta) = -x\sin(\theta) \le 0$ on $[0,\pi]$ while $(f'(\theta))^2 > 0$ on Ω_1. Thus

$$\left|\int_{\Omega_1}\frac{f''(\theta)}{(f'(\theta))^2}\sin(f(\theta))\,d\theta\right| \;\le\; -\int_{\Omega_1}\frac{f''(\theta)}{(f'(\theta))^2}\,d\theta \;=\; \left[\frac{1}{f'(\theta)}\right]_{\partial\Omega_1}.$$

Furthermore $f'(\theta)$ is decreasing on $[0,\pi]$ so Ω_0 consists of a single interval. Hence $\partial\Omega_1\backslash\{0,\pi\}$ contains at most 2 points. Since $f(0) = 0$ and $f(\pi) = -n\pi$ we then get

$$|I_1| \;\le\; \left|\left[\frac{\sin(f(\theta))}{f'(\theta)}\right]_{\partial\Omega_1}\right| + \left[\frac{1}{f'(\theta)}\right]_{\partial\Omega_1} \;\le\; 6\max_{\theta\in\Omega_1}\frac{1}{|f'(\theta)|} \;\le\; 6x^{-1/2}. \tag{16}$$

Combining (15), (16) we now get

$$|J_n(x)| \;\le\; \frac{1}{\pi}\big(|I_0| + |I_1|\big) \;\le\; \frac{1}{\pi}\Big(\frac{4\pi}{3} + 6\Big)x^{-1/2} \;\le\; 4x^{-1/2},$$

completing the result. ∎

Lemma 2.6. *Suppose* $k' \ge 2$, $0 \le k' - k \le \rho(k'+k+1)^{1/2}$ *and* $2\rho \le (k'+k+1)^{1/6}$. *Then*

$$|U_{\mathbf{a}}^{k,k'}| \;\le\; \big(4(2\rho)^{-1/2} + \tfrac{1}{2}(2\rho)^2\big)\,(k'+k+1)^{-1/4}.$$

Before starting, note that as a clear consequence of (14) we have

$$|J_n(x)| \;\le\; 1. \tag{17}$$

Proof. Since $2, k \le k'$

$$k' - k \ \le\ \frac{1}{2}(k' + k + 1)^{2/3} \ \le\ \frac{1}{2}\Big(\frac{5}{2}\Big)^{2/3} k'^{2/3} \ \le\ k'^{2/3}.$$

Now combining (13) with (11), (17) and Lemmas 2.2 and 2.3 we get

$$\begin{aligned}
|U_{\mathbf{a}}^{k,k'}| \ &\le\ \sqrt{F_{k',k}} \sum_{j=0}^{\infty} |A_j| \, \frac{\rho^j}{(k'+k+1)^{j/2}} \, \big|J_{k'-k+j}\big(2\rho\sqrt{k'+k+1}\big)\big| \\
&\le\ \big|J_{k'-k}\big(2\rho\sqrt{k'+k+1}\big)\big| + \sum_{j\ge 2}^{\infty} \rho^j (k'+k+1)^{-j/6} \\
&\le\ \big|J_{k'-k}\big(2\rho\sqrt{k'+k+1}\big)\big| + \tfrac{1}{2}(2\rho)^2 (k'+k+1)^{-1/3},
\end{aligned}$$

where the last line follows from the hypothesis that $\rho(k'+k+1)^{-1/6} \le 1/2$. Lemma 2.5 can now be used to estimate the remaining Bessel function term. ■

Main estimate

The next result is the main estimate we will need for the matrix elements $|\langle V\phi_k, \phi_{k'}\rangle|$. This estimate is valid in a parabolic region around the diagonal $k = k'$; the width of this region is governed by the quantity

$$\gamma \ :=\ \min_{\mathbf{a}\in\Lambda'} |\mathbf{a}|_\alpha \,,$$

which is positive since Λ' is discrete and doesn't contain $\mathbf{0}$. Although not required in this paper, we remark that for a general parabolic region around the diagonal one is restricted to estimates of the form $|\langle V\phi_k, \phi_{k'}\rangle| \le C(V)(k'+k+1)^{-1/6}$.

Proposition 2.7. *Suppose V satisfies condition (5) and set*

$$\kappa \ =\ \min\{1/3, \gamma/(2\sqrt{3})\}. \tag{18}$$

If $n \in \mathbb{N}$ and $k, k' \in \mathbb{N}_0$ satisfy $|k-n|, |k'-n| \le \kappa n^{1/2}$ then

$$|\langle V\phi_k, \phi_{k'}\rangle| \ \le\ C(V)\, n^{-1/4}. \tag{19}$$

Proof. We have $|\langle V\phi_k, \phi_{k'}\rangle| \le \|V\|$ for any $k, k' \in \mathbb{N}_0$ so we can increase $C(V)$ if necessary to ensure that (19) is satisfied for $n = 1, 2$. Furthermore V is self-adjoint so $|\langle V\phi_{k'}, \phi_k\rangle| = |\langle V\phi_k, \phi_{k'}\rangle|$. It thus suffices to prove the result assuming $n \ge 3$ and $k', k \in \mathbb{N}_0$ satisfy $k' \ge k$ and $|k-n|, |k'-n| \le \kappa n^{1/2}$. Then $k', k \ge n - \frac{1}{3}n^{1/2} \ge \frac{2}{3}n$ so $k' \ge 2$,

$$k' + k + 1 \ \ge\ \frac{4}{3}n \tag{20}$$

and

$$0 \;\le\; k' - k \;\le\; 2\kappa n^{1/2} \;\le\; \frac{\gamma}{2}(k' + k + 1)^{1/2}. \tag{21}$$

Now set $K = (k' + k + 1)^{1/6}$. Using (2), (7) and (8) we have

$$|\langle V\phi_k, \phi_{k'}\rangle| \;\le\; \sum_{\mathbf{a}\in\Lambda'} |U_{\mathbf{a}}^{k,k'}||V_{\mathbf{a}}| \;\le\; \sum_{\substack{\mathbf{a}\in\Lambda' \\ |\mathbf{a}|_\alpha \le K}} |U_{\mathbf{a}}^{k,k'}||V_{\mathbf{a}}| + \sum_{\substack{\mathbf{a}\in\Lambda' \\ |\mathbf{a}|_\alpha > K}} |V_{\mathbf{a}}|. \tag{22}$$

Since $1 < K^{-3/2}|\mathbf{a}|_\alpha^{3/2}$ whenever $|\mathbf{a}|_\alpha > K$, (5) and (20) give us

$$\sum_{\substack{\mathbf{a}\in\Lambda' \\ |\mathbf{a}|_\alpha > K}} |V_{\mathbf{a}}| \;\le\; K^{-3/2}\sum_{\mathbf{a}\in\Lambda'} |\mathbf{a}|_\alpha^{3/2}|V_{\mathbf{a}}| \;\le\; C(V)\,n^{-1/4}.$$

Now let $\mathbf{a} \in \Lambda'$. Since $|\mathbf{a}|_\alpha = 2\rho$ (see (10)) the definition of γ implies $\gamma/2 \le \rho$ and thus $k' - k \le \rho K^3$ by (21). Lemma 2.6, (5) and (20) then give

$$\sum_{\substack{\mathbf{a}\in\Lambda' \\ |\mathbf{a}|_\alpha \le K}} |U_{\mathbf{a}}^{k,k'}||V_{\mathbf{a}}| \;\le\; K^{-3/2}\sum_{\mathbf{a}\in\Lambda'} (4|\mathbf{a}|_\alpha^{-1/2} + \tfrac{1}{2}|\mathbf{a}|_\alpha^2)\,|V_{\mathbf{a}}| \;\le\; C(V)\,n^{-1/4}.$$

The result follows. ∎

First order term

The next result is used to obtain the explicit form for the first order correction term in the asymptotics for $\lambda_n(H + V)$.

Proposition 2.8. *Suppose V satisfies condition* (5)*. Then*

$$\langle V\phi_n, \phi_n\rangle \;=\; W(\sqrt{n})\,n^{-1/4} + O(n^{-1/2})$$

as $n \to +\infty$, where W is defined by (6)*.*

Proof. Let $\mathbf{a} \in T^*\mathbb{R}\backslash\{\mathbf{0}\}$ and set $\rho = |\mathbf{a}|_\alpha/2$. Using (13) and the fact that $F_{n,n} = 1$ we get

$$U_{\mathbf{a}}^{n,n} \;=\; \sum_{j=0}^{\infty} A_j\,\frac{\rho^j}{(2n+1)^{j/2}}\,J_j\big(2\rho\sqrt{2n+1}\big).$$

Now suppose $2\rho \le N$ where $N := (2n+1)^{1/6}$. Using (11), (17) and Lemma 2.2 we have

$$\begin{aligned}\big|U_{\mathbf{a}}^{n,n} - J_0(2\rho\sqrt{2n+1})\big| \;&\le\; \tfrac{1}{2}\rho^2(2n+1)^{-1} + \sum_{j\ge 3}\rho^j(2n+1)^{-j/6} \\ &\le\; \tfrac{1}{8}|\mathbf{a}|_\alpha^2(2n+1)^{-1} + \tfrac{1}{4}|\mathbf{a}|_\alpha^3(2n+1)^{-1/2}.\end{aligned}$$

Standard asymptotic forms for Bessel functions (see 9.2.1 in [AS]) give us

$$J_0(z) \;=\; \sqrt{\frac{2}{\pi z}}\cos\Big(z-\frac{\pi}{4}\Big)+O(z^{-3/2})$$

while

$$\left|\frac{d}{dz}\Big(\frac{1}{\sqrt{z}}\cos\Big(z-\frac{\pi}{4}\Big)\Big)\right| \;\le\; z^{-1/2}+\frac{1}{2}z^{-3/2}$$

and $2\rho\sqrt{2n+1}-2\rho\sqrt{2n}\le 2^{-1/2}\rho n^{-1/2}$. It follows that

$$\begin{aligned}
&\left|J_0(2\rho\sqrt{2n+1})-\sqrt{\frac{2}{\pi}}(2\rho)^{-1/2}(2n)^{-1/4}\cos\Big(2\rho\sqrt{2n}-\frac{\pi}{4}\Big)\right|\\
&\qquad\le\; C(2\rho)^{-3/2}(2n+1)^{-3/4}\\
&\qquad\qquad\quad+\sqrt{\frac{2}{\pi}}\Big((2\rho)^{-1/2}(2n)^{-1/4}+\frac{1}{2}(2\rho)^{-3/2}(2n)^{-3/4}\Big)\,2^{-1/2}\rho n^{-1/2}\\
&\qquad\le\; C((2\rho)^{-3/2}+(2\rho)^{1/2})n^{-3/4}.
\end{aligned}$$

Combining the above estimates we thus obtain

$$\left|U_{\mathbf{a}}^{n,n}-\frac{2^{1/4}}{\sqrt{\pi}}|\mathbf{a}|_\alpha^{-1/2}n^{-1/4}\cos\Big(|\mathbf{a}|_\alpha\sqrt{2n}-\frac{\pi}{4}\Big)\right| \;\le\; C(|\mathbf{a}|_\alpha^{-3/2}+|\mathbf{a}|_\alpha^{3})n^{-1/2}$$

whenever $|\mathbf{a}|_\alpha\le N$. Using (2), (6), (7) and (8) we thus have

$$\begin{aligned}
&\big|\langle V\phi_n,\phi_n\rangle - W(\sqrt{n})n^{-1/4}\big|\\
&\qquad\le\; Cn^{-1/2}\sum_{\substack{\mathbf{a}\in\Lambda'\\|\mathbf{a}|_\alpha\le N}}(|\mathbf{a}|_\alpha^{-3/2}+|\mathbf{a}|_\alpha^{3})\,|V_{\mathbf{a}}|+\sum_{\substack{\mathbf{a}\in\Lambda'\\|\mathbf{a}|_\alpha> N}}(1+|\mathbf{a}|_\alpha^{-1/2})|V_{\mathbf{a}}|.
\end{aligned}$$

Since $1<N^{-3}|\mathbf{a}|_\alpha^3<n^{-1/2}|\mathbf{a}|_\alpha^3$ whenever $|\mathbf{a}|_\alpha>N$ the term inside the last sum can be replaced with $n^{-1/2}(|\mathbf{a}|_\alpha^3+|\mathbf{a}|_\alpha^{5/2})|V_{\mathbf{a}}|$. Using (5) we then get

$$\big|\langle V\phi_n,\phi_n\rangle - W(\sqrt{n})n^{-1/4}\big| \;\le\; Cn^{-1/2}\sum_{\mathbf{a}\in\Lambda'}(|\mathbf{a}|_\alpha^{-3/2}+|\mathbf{a}|_\alpha^{3})\,|V_{\mathbf{a}}| \;\le\; C(V)n^{-1/2},$$

completing the result. ∎

3 Resolvent Estimates

For any $\lambda\in\mathbb{C}\backslash\sigma(H)$ let $R(\lambda)\;=\;(H-\lambda)^{-1}$ denote the resolvent of the operator H; we will also write R for $R(\lambda)$ where this should not cause confusion.

Let κ denote the constant defined in (18). For a given $n \in \mathbb{N}$ we will make repeated use of the partition of $\mathbb{N}_0$ defined by

$$I = \left\{k \in \mathbb{N}_0 \,\middle|\, |k-n| \le \kappa n^{1/2}\right\} \quad \text{and} \quad J = \mathbb{N}_0 \backslash I. \tag{23}$$

For any $\varepsilon \in (0,\alpha)$ and $n \in \mathbb{N}_0$, let $\Gamma_{\varepsilon,n}$ be the anti-clockwise circular contour in $\mathbb{C}$ centred at $\lambda_n = \lambda_n(H) = \alpha(2n+1)$. If $\lambda \in \Gamma_{\varepsilon,n}$ then $\lambda = \alpha(2n+1) + \varepsilon e^{i\theta}$ for some $\theta \in [0,2\pi)$. It follows that $|\lambda - \lambda_k| = |2\alpha(n-k) + \varepsilon e^{i\theta}|$ for any $k \in \mathbb{N}_0$. Straightforward arguments then lead to the following estimates;

$$\sum_{k\in I} |\lambda - \lambda_k|^{-1} \;\le\; C(\varepsilon)\,\ln(n), \tag{24}$$

$$\sum_{k\in \mathbb{N}_0} |\lambda - \lambda_k|^{-2} \;\le\; C(\varepsilon), \tag{25}$$

$$\sum_{k\in J} |\lambda - \lambda_k|^{-2} \;\le\; C n^{-1/2} \tag{26}$$

and

$$|\lambda - \lambda_k| \ge C n^{1/2} \quad \text{for any } k \in J. \tag{27}$$

The first two results in this section relate to the operator $R(\lambda)VR(\lambda)$, which is clearly bounded whenever λ is in the resolvent set of H. We show that it is in fact trace class while its operator norm decreases as $n^{-1/4}$ for $\lambda \in \Gamma_{\varepsilon,n}$.

Lemma 3.1. *For any $n \in \mathbb{N}$ and $\lambda \in \Gamma_{\varepsilon,n}$ we have*

$$\|R(\lambda)VR(\lambda)\| \;\le\; \|R(\lambda)VR(\lambda)\|_2 \;\le\; C(V,\varepsilon)\, n^{-1/4}.$$

We remark that since $\{\phi_k \,|\, k \in \mathbb{N}_0\}$ is an orthonormal basis of $L^2(\mathbb{R})$

$$\sum_{k'\in \mathbb{N}_0} |\langle V\phi_k, \phi_{k'}\rangle|^2 \;=\; \|V\phi_k\|^2 \;\le\; \|V\|^2. \tag{28}$$

Proof. Using the orthonormal basis $\{\phi_k \,|\, k \in \mathbb{N}_0\}$ we have

$$\|RVR\|_2^2 \;=\; \sum_{k,k'\in\mathbb{N}_0} |\langle RVR\phi_k, \phi_{k'}\rangle|^2 \;=\; \sum_{k,k'\in\mathbb{N}_0} \frac{|\langle V\phi_k, \phi_{k'}\rangle|^2}{|\lambda_k - \lambda|^2 |\lambda_{k'} - \lambda|^2}. \tag{29}$$

We will split this sum using the partition (23). Firstly Proposition 2.7 and (25) imply

$$\sum_{k,k'\in I} \frac{|\langle V\phi_k, \phi_{k'}\rangle|^2}{|\lambda_k - \lambda|^2 |\lambda_{k'} - \lambda|^2} \;\le\; C(V) n^{-1/2} \Bigg(\sum_{k\in I} \frac{1}{|\lambda_k - \lambda|^2} \Bigg)^2 \;\le\; C(V,\varepsilon) n^{-1/2}.$$

Now using (27), (28) and (25) we get

$$\sum_{\substack{k\in\mathbb{N}_0\\ k'\in J}} \frac{|\langle V\phi_k,\phi_{k'}\rangle|^2}{|\lambda_k-\lambda|^2|\lambda_{k'}-\lambda|^2} \;\le\; Cn^{-1}\sum_{k\in\mathbb{N}_0}\frac{1}{|\lambda_k-\lambda|^2}\sum_{k'\in J}|\langle V\phi_k,\phi_{k'}\rangle|^2$$
$$\le\; C(V,\varepsilon)n^{-1}.$$

The remaining part of the sum on the right hand side of (29) involves $k\in J$ and $k'\in I\subset\mathbb{N}_0$; thus we can estimate this part using an argument similar to the last one with k and k' swapped. ■

Lemma 3.2. *For any $n\in\mathbb{N}_0$ and $\lambda\in\Gamma_{\varepsilon,n}$ the operator $R(\lambda)VR(\lambda)$ is trace class. Furthermore $\|R(\lambda)VR(\lambda)\|_1$ is uniformly bounded (in n and $\lambda\in\Gamma_{\varepsilon,n}$).*

Proof. The set $\{\phi_k\,|\,k\in\mathbb{N}_0\}$ is an orthonormal eigenbasis for R with corresponding eigenvalues $(\lambda_k-\lambda)^{-1}$, $k\in\mathbb{N}_0$ so (25) implies

$$\|R\|_2^2 \;=\; \sum_{k\in\mathbb{N}_0}|\lambda_k-\lambda|^{-2} \;\le\; C(\varepsilon).$$

Thus $\|RVR\|_1 \;=\; \|VR^2\|_1 \;\le\; \|V\|\,\|R^2\|_1 \;\le\; \|V\|\,\|R\|_2^2 \;\le\; C(\varepsilon)\,\|V\|$. ■

Suppose $n\in\mathbb{N}_0$ and $j\in\mathbb{N}$. From the previous result we know that $R(\lambda)VR(\lambda)$ is trace class for any $\lambda\in\Gamma_{\varepsilon,n}$. On the other hand $R(\lambda)V$ is bounded (in fact $\|R(\lambda)V\|\le\varepsilon^{-1}\|V\|$). It follows that

$$(R(\lambda)V)^jR(\lambda) \;=\; (R(\lambda)V)^{j-1}R(\lambda)VR(\lambda)$$

is also trace class with trace norm uniformly bounded for $\lambda\in\Gamma_{\varepsilon,n}$. The work in the remainder of this section leads to Proposition 3.5 where we obtain an estimate for the trace of an integral of such operators.

Lemma 3.3. *Let $n\ge 2$, $\lambda\in\Gamma_{\varepsilon,n}$ and suppose $f:\mathbb{N}_0\to\mathbb{C}$ satisfies*

$$\sum_{k\in\mathbb{N}_0}|f(k)|^2 \;\le\; C_1^2 \quad \text{and} \quad |f(k)| \;\le\; C_1n^{-1/4} \text{ when } k\in I \tag{30}$$

for some constant C_1. For each $k\in\mathbb{N}_0$ set

$$g(k) = \sum_{k'\in\mathbb{N}_0}\frac{f(k')\,\langle V\phi_{k'},\phi_k\rangle}{\lambda-\lambda_{k'}}.$$

Then there exists a constant $K=K(V,\varepsilon)$ such that

$$\sum_{k\in\mathbb{N}_0}|g(k)|^2 \;\le\; C_1^2K^2n^{-1/2}\ln^2(n) \quad \text{and} \quad |g(k)| \;\le\; C_1Kn^{-1/2}\ln(n) \text{ when } k\in I.$$

Proof. Since

$$\sum_{k\in\mathbb{N}_0} |g(k)|^2 \;=\; \sum_{k,k',k''\in\mathbb{N}_0} \frac{f(k')\overline{f(k'')}\langle V\phi_{k'},\phi_k\rangle\langle\phi_k,V\phi_{k''}\rangle}{(\lambda-\lambda_{k'})\overline{(\lambda-\lambda_{k''})}}$$

and

$$\Big|\sum_{k\in\mathbb{N}_0}\langle V\phi_{k'},\phi_k\rangle\langle\phi_k,V\phi_{k''}\rangle\Big| \;=\; \big|\langle V\phi_{k'},V\phi_{k''}\rangle\big| \;\le\; \|V\|^2$$

it follows that

$$\sum_{k\in\mathbb{N}_0}|g(k)|^2 \;\le\; \|V\|^2\Big(\sum_{k\in I}\frac{|f(k)|}{|\lambda-\lambda_k|} + \sum_{k\in J}\frac{|f(k)|}{|\lambda-\lambda_k|}\Big)^2.$$

Using the second part of (30) and (24) we get

$$\sum_{k\in I}\frac{|f(k)|}{|\lambda-\lambda_k|} \;\le\; C_1 n^{-1/4}\sum_{k\in I}|\lambda-\lambda_k|^{-1} \;\le\; C_1C_2(\varepsilon)n^{-1/4}\ln(n).$$

On the other hand the first part of (30) and (26) give

$$\begin{aligned}\sum_{k\in J}\frac{|f(k)|}{|\lambda-\lambda_k|} \;&\le\; \Big(\sum_{k\in J}|f(k)|^2\Big)^{1/2}\Big(\sum_{k\in J}|\lambda-\lambda_k|^{-2}\Big)^{1/2}\\ &\le\; C_1C_3n^{-1/4} \;\le\; 2C_1C_3n^{-1/4}\ln(n).\end{aligned}$$

Putting these estimates together now leads to

$$\sum_{k\in\mathbb{N}_0}|g(k)|^2 \;\le\; C_1^2K_1^2n^{-1/2}\ln^2(n),$$

with $K_1 = \|V\|(C_2(\varepsilon)+2C_3)$. Now suppose $k\in I$ and write $g(k) = g_I(k)+g_J(k)$ where

$$g_I(k) = \sum_{k'\in I}\frac{f(k')\,\langle V\phi_{k'},\phi_k\rangle}{\lambda-\lambda_{k'}} \quad\text{and}\quad g_J(k) = \sum_{k'\in J}\frac{f(k')\,\langle V\phi_{k'},\phi_k\rangle}{\lambda-\lambda_{k'}}.$$

From Proposition 2.7, the second part of (30) and (24) we get

$$|g_I(k)| \;\le\; C_1C(V)n^{-1/2}\sum_{k'\in I}|\lambda-\lambda_{k'}|^{-1} \;\le\; C_1C_4(V,\varepsilon)\,n^{-1/2}\ln(n).$$

On the other hand (27), the first part of (30) and (28) give us

$$\begin{aligned}|g_J(k)| \;&\le\; C(\varepsilon)n^{-1/2}\Big(\sum_{k'\in J}|f(k')|^2\Big)^{1/2}\Big(\sum_{k'\in J}\big|\langle V\phi_{k'},\phi_k\rangle\big|^2\Big)^{1/2}\\ &\le\; C_1C_5(\varepsilon)\|V\|n^{-1/2} \;\le\; 2C_1C_5(\varepsilon)\|V\|n^{-1/2}\ln(n).\end{aligned}$$

Putting these estimates together now leads to $|g(k)|\le C_1K_2n^{-1/2}\ln(n)$ with $K_2 = C_4(V,\varepsilon)+2C_5(\varepsilon)\|V\|$. Taking $K=\max\{K_1,K_2\}$, completes the result. ■

Taking $f(k) = \langle V\phi_n, \phi_k\rangle$ we can use (28) and Proposition 2.7 to check that (30) is satisfied. The next result then follows from Lemma 3.3 by use of induction; we can take $K = \max\{\|V\|, C(V), K'\}$ where $C(V)$ and K' are the constants coming from Proposition 2.7 and Lemma 3.3 respectively.

Lemma 3.4. *Suppose $n \geq 2$ and $j \in \mathbb{N}_0$. Then there exists a constant $K = K(V, \varepsilon)$ such that for all $\lambda \in \Gamma_{\varepsilon,n}$ we have*

$$\left| \sum_{k_1,\dots,k_j \in \mathbb{N}_0} \frac{\langle V\phi_n, \phi_{k_1}\rangle \langle V\phi_{k_1}, \phi_{k_2}\rangle \dots \langle V\phi_{k_j}, \phi_n\rangle}{(\lambda - \lambda_{k_1}) \dots (\lambda - \lambda_{k_j})} \right| \;\leq\; K^{j+1} n^{-(j+1)/4} \ln^j(n).$$

Proposition 3.5. *Suppose $n \geq 2$ and $j \in \mathbb{N}$. Then*

$$\left| \operatorname{Tr} \frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon,n}} \lambda\, R(\lambda)(VR(\lambda))^j \, d\lambda \right| \;\leq\; K^j n^{-j/4} \ln^{j-1}(n),$$

where K is the constant from Lemma 3.4.

Proof. Since $\{\phi_{k'} \mid k' \in \mathbb{N}_0\}$ is an orthonormal basis of $L^2(\mathbb{R})$ we have

$$(VR)\phi_k \;=\; \sum_{k' \in \mathbb{N}_0} \langle VR\phi_k, \phi_{k'}\rangle \phi_{k'} \;=\; \sum_{k' \in \mathbb{N}_0} \frac{\langle V\phi_k, \phi_{k'}\rangle}{\lambda_k - \lambda} \phi_{k'}.$$

Continuing by induction we get

$$(VR)^j \phi_k \;=\; \sum_{k_1,\dots,k_j \in \mathbb{N}_0} \frac{\langle V\phi_k, \phi_{k_1}\rangle \langle V\phi_{k_1}, \phi_{k_2}\rangle \dots \langle V\phi_{k_{j-1}}, \phi_{k_j}\rangle}{(\lambda_k - \lambda)(\lambda_{k_1} - \lambda) \dots (\lambda_{k_{j-1}} - \lambda)} \phi_{k_j}.$$

Together with the fact that $\langle R\phi_{k_j}, \phi_{k_0}\rangle = \delta_{k_j,k_0}(\lambda_{k_0} - \lambda)^{-1}$ we now get

$$\begin{aligned}
\operatorname{Tr}(R(VR)^j) \;&=\; \sum_{k_0 \in \mathbb{N}_0} \left\langle R(VR)^j \phi_{k_0}, \phi_{k_0} \right\rangle \\
&=\; \sum_{k_0,\dots,k_j \in \mathbb{N}_0} \frac{\langle V\phi_{k_0}, \phi_{k_1}\rangle \langle V\phi_{k_1}, \phi_{k_2}\rangle \dots \langle V\phi_{k_{j-1}}, \phi_{k_j}\rangle}{(\lambda_{k_0} - \lambda)(\lambda_{k_1} - \lambda) \dots (\lambda_{k_{j-1}} - \lambda)} \langle R\phi_{k_j}, \phi_{k_0}\rangle \\
&=\; \sum_{k_0,\dots,k_{j-1} \in \mathbb{N}_0} \frac{\langle V\phi_{k_0}, \phi_{k_1}\rangle \langle V\phi_{k_1}, \phi_{k_2}\rangle \dots \langle V\phi_{k_{j-1}}, \phi_{k_0}\rangle}{(\lambda_{k_0} - \lambda)^2 (\lambda_{k_1} - \lambda) \dots (\lambda_{k_{j-1}} - \lambda)} \;=\; \sum_{l=0}^{j-1} \frac{1}{\lambda_{k_l} - \lambda} A(\lambda),
\end{aligned}$$

where $A(\lambda)$ is the meromorphic function

$$A(\lambda) \;=\; \frac{1}{j} \sum_{k_0,\dots,k_{j-1} \in \mathbb{N}_0} \frac{\langle V\phi_{k_0}, \phi_{k_1}\rangle \langle V\phi_{k_1}, \phi_{k_2}\rangle \dots \langle V\phi_{k_{j-1}}, \phi_{k_0}\rangle}{(\lambda_{k_0} - \lambda)(\lambda_{k_1} - \lambda) \dots (\lambda_{k_{j-1}} - \lambda)}. \tag{31}$$

Since

$$\frac{d}{d\lambda}\lambda\Big(\prod_{i=0}^{j-1}\frac{1}{\lambda_{k_i}-\lambda}\Big) \;=\; \prod_{i=0}^{j-1}\frac{1}{\lambda_{k_i}-\lambda} + \lambda\sum_{l=0}^{j-1}\frac{1}{\lambda_{k_l}-\lambda}\Big(\prod_{i=0}^{j-1}\frac{1}{\lambda_{k_i}-\lambda}\Big)$$

for any $k_0,\dots,k_{j-1}\in\mathbb{N}_0$, we can rewrite the above equation as

$$\mathrm{Tr}\;\lambda R(VR)^j \;=\; \frac{d}{d\lambda}\big(\lambda A(\lambda)\big) - A(\lambda).$$

Integrating around the contour $\Gamma_{\varepsilon,n}$ it follows that

$$\mathrm{Tr}\;\frac{1}{2\pi i}\oint_{\Gamma_{\varepsilon,n}}\lambda R(VR)^j\,d\lambda \;=\; -\frac{1}{2\pi i}\oint_{\Gamma_{\varepsilon,n}}A(\lambda)\,d\lambda. \tag{32}$$

The poles of the meromorphic function $A(\lambda)$ occur at the points $\lambda=\lambda_k$ for $k\in\mathbb{N}_0$. Since the only such point enclosed by the contour $\Gamma_{\varepsilon,n}$ is $\lambda=\lambda_n$, it follows that the only terms in the series (31) which contribute to the right hand side of (32) are those with at least one of $k_0,\dots,k_{j-1}$ equal to n. With the help of symmetry we then obtain the identity

$$\begin{aligned}&\mathrm{Tr}\;\frac{1}{2\pi i}\oint_{\Gamma_{\varepsilon,n}}\lambda R(VR)^j\,d\lambda\\ &= \;-\frac{1}{2\pi i}\oint_{\Gamma_{\varepsilon,n}}\frac{1}{\lambda_n-\lambda}\sum_{k_1,\dots,k_{j-1}\in\mathbb{N}_0}\frac{\langle V\phi_n,\phi_{k_1}\rangle\langle V\phi_{k_1},\phi_{k_2}\rangle\dots\langle V\phi_{k_{j-1}},\phi_n\rangle}{(\lambda_{k_1}-\lambda)\dots(\lambda_{k_{j-1}}-\lambda)}\,d\lambda.\end{aligned} \tag{33}$$

For any $\lambda\in\Gamma_{\varepsilon,n}$ we have $|\lambda_n-\lambda|=\varepsilon$ while

$$\left|\sum_{k_1,\dots,k_{j-1}\in\mathbb{N}_0}\frac{\langle V\phi_n,\phi_{k_1}\rangle\langle V\phi_{k_1},\phi_{k_2}\rangle\dots\langle V\phi_{k_{j-1}},\phi_n\rangle}{(\lambda_{k_1}-\lambda)\dots(\lambda_{k_{j-1}}-\lambda)}\right| \;\le\; K^j n^{-j/4}\ln^{j-1}(n)$$

by Lemma 3.4. Since the length of $\Gamma_{\varepsilon,n}$ is $2\pi\varepsilon$ we finally get

$$\left|\mathrm{Tr}\;\frac{1}{2\pi i}\oint_{\Gamma_{\varepsilon,n}}\lambda R(VR)^j\,d\lambda\right| \;\le\; \frac{1}{2\pi}\oint_{\Gamma_{\varepsilon,n}}\frac{1}{\varepsilon}K^j n^{-j/4}\ln^{j-1}(n)\,d\lambda \;=\; K^j n^{-j/4}\ln^{j-1}(n),$$

completing the result. ∎

Taking $j=1$ in (33) leads to the formula

$$\begin{aligned}&\mathrm{Tr}\;\frac{1}{2\pi i}\oint_{\Gamma_{\varepsilon,n}}\lambda R(\lambda)VR(\lambda)\,d\lambda\\ &\qquad= -\frac{1}{2\pi i}\oint_{\Gamma_{\varepsilon,n}}\frac{1}{\lambda_n-\lambda}\langle V\phi_n,\phi_n\rangle\,d\lambda \;=\; \langle V\phi_n,\phi_n\rangle.\end{aligned} \tag{34}$$

This is needed to obtain the first order correction term in Theorem 1.1.

4 Proof of Theorem 1.1

Lemmas 3.1 and 3.2 give us $\|R(\lambda)VR(\lambda)\| \leq C_1 n^{-1/4}$ and $\|R(\lambda)VR(\lambda)\|_1 \leq C_2$ for all $n \in \mathbb{N}$ and $\lambda \in \Gamma_{\varepsilon,n}$. In particular $\|(VR(\lambda))^2\| \leq \|V\| C_1 n^{-1/4}$. We also note that $\|R(\lambda)\| = \varepsilon^{-1}$. It follows that for any $j \in \mathbb{N}_0$ we get

$$\|(VR(\lambda))^{2j}\| \;\leq\; \|(VR(\lambda))^2\|^j \;\leq\; (\|V\|C_1 n^{-1/4})^j$$

and

$$\|(VR(\lambda))^{2j+1}\| \;\leq\; \|V\|\|R(\lambda)\|\|(VR(\lambda))^{2j}\| \;\leq\; \|V\|\varepsilon^{-1}(\|V\|C_1 n^{-1/4})^j.$$

Choose $N' \in \mathbb{N}$ so that $\|V\|C_1 N'^{-1/4} \leq 1/2$. It follows that for any $n \geq N'$ and $\lambda \in \Gamma_{\varepsilon,n}$ the series

$$(I + VR(\lambda))^{-1} \;=\; \sum_{j=0}^{\infty} (-VR(\lambda))^j \tag{35}$$

is absolutely convergent and has norm bounded by $2(1 + \|V\|\varepsilon^{-1})$. In particular, $I + VR(\lambda)$ is invertible with a uniformly bounded inverse for all $n \geq N'$ and $\lambda \in \Gamma_{\varepsilon,n}$. On the other hand, the series

$$T(\lambda) \;:=\; \sum_{j=1}^{\infty} R(\lambda)(-VR(\lambda))^j \;=\; -R(\lambda)VR(\lambda)\sum_{j=0}^{\infty}(-VR(\lambda))^j$$

is convergent in trace class with

$$\|T(\lambda)\|_1 \;\leq\; \|R(\lambda)VR(\lambda)\|_1 \, \|(I + VR(\lambda))^{-1}\| \;\leq\; 2C_2(1 + \|V\|\varepsilon^{-1})$$

for $n \geq N'$ and $\lambda \in \Gamma_{\varepsilon,n}$. Setting

$$T_n \;=\; -\frac{1}{2\pi i}\oint_{\Gamma_{\varepsilon,n}} \lambda T(\lambda)\, d\lambda$$

it follows that we have an absolutely convergent expansion

$$\operatorname{Tr} T_n \;=\; -\sum_{j=1}^{\infty} \operatorname{Tr} \frac{1}{2\pi i}\oint_{\Gamma_{\varepsilon,n}} \lambda R(\lambda)(-VR(\lambda))^j \, d\lambda$$

whenever $n \geq N'$.

Now choose $N \geq N'$ so that $KN^{-1/4}\ln(N) \leq 1/2$ where K is the constant given by Proposition 3.5. Using this Proposition and the above results it follows that

$$\left|\sum_{j=2}^{\infty} \operatorname{Tr} \frac{1}{2\pi i}\oint_{\Gamma_{\varepsilon,n}} \lambda R(\lambda)(-VR(\lambda))^j \, d\lambda\right| \;\leq\; 2K^2 n^{-1/2}\ln(n)$$

for all $n \geq N$. Therefore

$$\begin{aligned}
\operatorname{Tr} T_n &= \operatorname{Tr} \frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon,n}} \lambda R(\lambda) V R(\lambda)\, d\lambda \,+\, O(n^{-1/2} \ln(n)) \\
&= \langle V\phi_n, \phi_n \rangle \,+\, O(n^{-1/2} \ln(n))
\end{aligned}$$

for all $n \geq N$, where we have used (34).

The argument can be tied together using a standard resolvent expansion. Set $R_V(\lambda) = (H + V - \lambda)^{-1}$ and let $n \geq N$. Then

$$R_V(\lambda) \;=\; R(\lambda)(1 + VR(\lambda))^{-1} \;=\; R(\lambda) \sum_{j=0}^{\infty} (-VR(\lambda))^j.$$

The right hand side of (35) will still converge if V is replaced with gV for some $g \in [0, 1]$. Hence $\sigma(H + gV) \cap \Gamma_{\varepsilon,n} = \emptyset$. Since the eigenvalues of $H + gV$ depend continuously on g, it follows that $\Gamma_{\varepsilon,n}$ must enclose $\lambda_n(H + V)$ but no other points of $\sigma(H + V)$. Thus we can write

$$\begin{aligned}
\lambda_n(H + V) - \lambda_n(H) &= -\frac{1}{2\pi i} \operatorname{Tr} \oint_{\Gamma_{\varepsilon,n}} \lambda (R_V(\lambda) - R(\lambda))\, d\lambda \\
&= -\frac{1}{2\pi i} \operatorname{Tr} \oint_{\Gamma_{\varepsilon,n}} \lambda \sum_{j=1}^{\infty} R(\lambda)(-VR(\lambda))^j \, d\lambda \\
&= \operatorname{Tr} T_n \;=\; \langle V\phi_n, \phi_n \rangle + O(n^{-1/2} \ln(n)).
\end{aligned}$$

Theorem 1.1 now follows from Proposition 2.8.

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